Propagation of Neutron Cross Section, Fission Yield, and Decay Data Uncertainties in Depletion Calculations

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Propagation of nuclear data uncertainties in reactor calculations is interesting for design purposes and libraries evaluation. Previous versions of the GRS XSUSA library propagated only neutron cross section uncertainties. We have extended XSUSA uncertainty assessment capabilities by including propagation of fission yields and decay data uncertainties due to the their relevance in depletion simulations. We apply this extended methodology to the UAM6 PWR Pin-Cell Burnup Benchmark, which involves uncertainty propagation through burnup.

I. INTRODUCTION

Characterization of nuclear systems through simulation codes should be supplemented by an assessment of the associated uncertainties stemming from experimental and data evaluation processes. Besides engineering and operational data, nuclear libraries are a source of uncertainty of high importance. XSUSA [1] propagates cross section uncertainties to the SCALE 6.1 [2] calculations. The methodology is based on the GRS method [3]: it employs a repetition of calculations, the inputs of which are variations of the original. These variations of the input data are randomly generated from the probability distributions of the parameters including possible correlations between them. After performing all the calculations (typically 100 or more), the output quantities are statistically analyzed and their uncertainty ranges and sensitivities with respect to the input parameters are determined. The GRS method with nuclear cross sections varies the master libraries in the appropriate group structure according to the uncertainty information in the covariance matrices for each nuclide/reaction combination considered, taking into account, if present, the covariances between different energy groups, different reactions, and different nuclides. The consistency of the resulting cross section set has to be assured before performing a series of calculations and finally performing the statistical analysis.

The method developed at GRS has been proved to be a useful tool in the propagation of cross section uncertainties to any system response, completing reactor physics calculations with uncertainty values arising from uncertainties in the nuclear data libraries. However, when performing depletion calculations, additional nuclear data sources play an important role: decay information and fission yields. Along with the cross sections calculated by the transport solvers, a depletion code (such as SCALE 6.1/ORIGEN-S) utilizes general decay information and specific fission yields data in order to complete the transition matrix involving all the physical processes that determine the isotopic evolution. These additional quantities are not free of uncertainty and, therefore, it must be well determined how they propagate to quantities such as criticality and isotopic concentrations, which is of high interest in detailed burnup credit calculations.

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II. METHODOLOGY

Propagation of fission yields and decay data uncertainties through depletion calculations following the XSUSA method requires a previous step focused on the generation of varied libraries. A varied value is generated by a random sampling around it, assuming a Gaussian distribution whose standard deviation corresponds to the uncertainty in the sampled quantity. Thus, to vary all the information contained in the nuclear data libraries (fission yields and decay data) not only the nominal values of the magnitudes are needed but also their uncertainties. SCALE6.1/ORIGEN-S employs its own decay and fission yields libraries, based on the ENDF/B-VII.1 [4] evaluation, and delivered along with the code package, also in ASCII version. The fission yield library is provided in an ENDF6-like format with the difference that it contains no yield uncertainty information. Written in its own format, the ORIGEN-S ASCII decay library contains half-life and branching ratios values but it also lacks information about their uncertainties. In order to create new libraries, samplings are performed around the nominal values stored in the ORIGEN-S libraries assuming the uncertainty that is stored in the ENDF/B-VII.1 evaluation. The corresponding code has been developed to create sets of varied libraries. Basically, when present for a given isotope, they take the nominal magnitudes from the ORIGEN-S libraries and the uncertainties from the ENDF/B-VII.1; based on this information, they create an input for the XSUSA module MEDUSA; MEDUSA performs the sampling and provides new nominal values for the sampled magnitudes; and, finally, our codes create the fission yields and decay libraries using the values calculated by MEDUSA. This process must be repeated to create a pool of varied ASCII libraries.

In the current version of our methodology, we vary the fission yields taking into account all the information available to date, that is, standard deviation as the uncertainty. Due to the lack of covariances for them, no correlations affecting fission yields are considered here. Regarding decay data, half-lives and branching ratios are sampled. For the branching ratios, two variation schemes have been adopted depending on the number of existing decay channels. When two decay modes are present, since they are anticorrelated, it is possible to perform a short of correlated sampling by varying one of them and correcting correspondingly the other one, maintaining this way their sum to unity. In case more decay branches are possible, a separate sampling of their branching ratios is carried out. Then, the resulting varied ratios are renormalized to their sum to preserve unity.

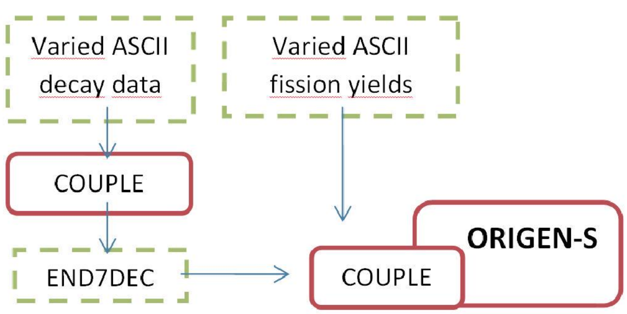

FIG. 1. Use of varied libraries by COUPLE and ORIGEN-S.

When running a depletion calculation, ORIGEN-S requires the AMPX working library containing cross sections, fission yields and decay data in binary format, created and updated by the SCALE module COUPLE from the ASCII files. Therefore, to study the impact of the fission yields and decay uncertainties in a depletion calculation, our fission yields and decay varied libraries must be called as ASCII input for COUPLE; this way, it creates a new decay binary library from the corresponding varied ASCII file and updates the working library using the varied fission yields. After their variation, both decay data and fission yields are correspondingly re-normalized. For two-mode decay processes, a total anticorrelation is applied. For multi-mode decay processes, a re-normalization to 1 is applied. For fission products, the re-normalization is to 2. Therefore, during the depletion, ORIGEN-S uses a binary library that contains the fission yields and decay info that result from our MEDUSA sampling according to the uncertainties contained in the ENDF/B-VII.1 library. This procedure, as sketched in Fig. 1 has been implemented and automated in the framework of the XSUSA package.

III. RESULTS

To test this methodology, a pin cell model is employed as defined in the UAM-LWR Benchmark Phase 1 (cf. Ref. [5]): a pure uranium pin cell with a ^{235}U enrichment of 4.85 %, burnt at a constant power of 33.58 MW/MTU during 1825 days, up to a final burnup of 61.28 GWd/MTU. After this irradiation period, the inventory decays during 300 years. The number of libraries generated beforehand is 1,000 for cross-sections, fission yields and decay libraries. Four sets of 1,000 depletion calculations each have been performed: first, varying only decay libraries; second, varying only fission yields; third, varying only cross-sections and, finally, varying them all at the same time in order to assess their joint impact.

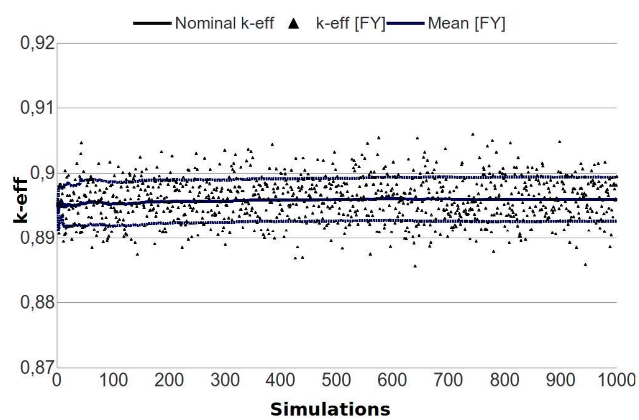

FIG. 2. k_{eff} values at end of irradiation from simulations using 1,000 varied fission yield libraries.

This set of calculations allows us to study the impact of the decay, fission yields and cross-section uncertainties on criticality at end of irradiation as well as their evolution in time. Figures 2 - 4 collect the results for the thousand criticality calculations at end of irradiation for each case. The uncertainties in decay data do not significantly impact the results: all the criticality values calculated at shutdown are practically identical to that from the nominal calculation, that is, the k_{eff} calculated from the original library. When varying the fission yield library, k_{eff} values scatter around the nominal one including it

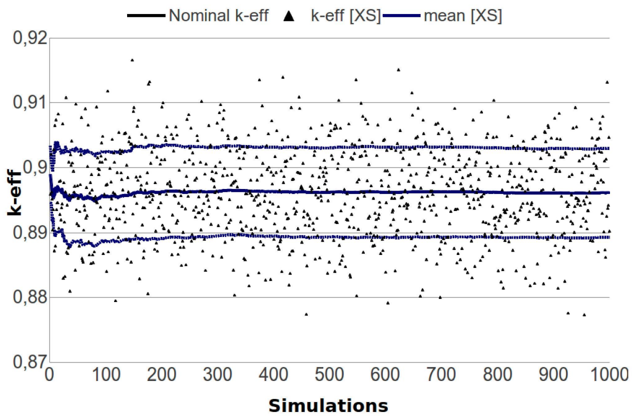

FIG. 3. k_{eff} values at end of irradiation from simulations using 1,000 varied cross section libraries.

within its error margins, as shown in Fig. 2. When varying the cross section data (Fig. 3), the scatter around the nominal value is substantially larger and yields the main contribution to the total uncertainty, as given in Fig. 4. Table I lists the nominal value of k_{eff} without uncertainty, averaged values and standard deviation for the thousand simulations varying the decay data, fision yields, cross sections and the three nuclear data together.

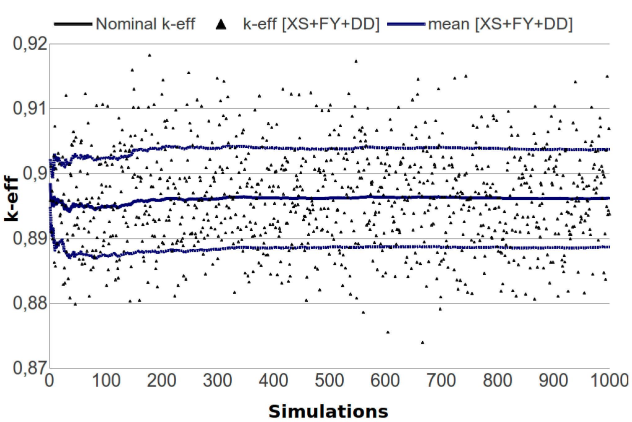

FIG. 4. k_{eff} values at end of irradiation from simulations using 1,000 varied nuclear data libraries (XS + FY + Decay).

TABLE I. Impact on k_{eff} from the sampling of the nuclear data sources at the end of irradiation time. Nominal value without uncertainty, averaged values and standard deviation for the thousand simulations varying nuclear data.

	k_{eff}	Uncertainty (pcm)
Nominal	0.89588	-
Decay	0.89588	1.05
Fission Yields	0.89601	376.0
Cross Sections	0.89613	763.0
All nuclear data	0.89623	841.0

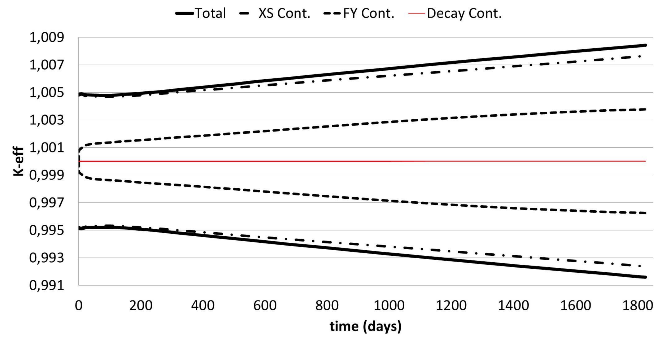

FIG. 5. k_{eff} values from simulations using 1,000 varied nuclear data libraries as a function of depletion time.

As can be seen, decay data implies a negligible uncertainty, especially when compared to fission yields and cross sections. This contribution profile, which is shown at the end of the depletion time, is maintained actually through the burnup. Figure 5 presents the relative error from the variation of the different nuclear data with burnup. It can be assessed the predominance of the cross-sections as uncertainty contributor at any time step, followed by fission products and decay data. It is important to note that there is an uncertainty increase with the irradiation time, clear for fission yields and cross sections, related to the larger amount of nuclides present at the modeled fuel. Table II shows the relative uncertainty values at the beginning and end of irradiation that arise from the variation of the different nuclear data libraries.

TABLE II. Relative uncertainty (in %) in k_{eff} at beginning and end of irradiation.

	t = 0 d	t = 1825 d
Decay	0.00	0.00
Fission Yields	0.00	0.38
Cross Sections	0.48	0.76
All nuclear data	0.48	0.84

When considering burnup credit calculations, one of the magnitudes of importance are the nuclide concentrations. Major actinides (uranium and plutonium isotopes) as well as some selected fission products (neodymium, samarium, cesium and technetium) are usual players in isotopic composition exercises. As a result of calculations based on nuclear data libraries, the prediction of these nuclides is affected by the nuclear data uncertainties. The uncertainty analysis of the major actinides and some fission products at the end of the cooling time provides the results shown in Table III. These relative uncertainty values are obtained as a result of the entire variation of the Decay, Fission Yields (FY), and Cross-Section (XS) libraries, both one by one and the three all at once (All). Uncertainties on the fission yields have a high impact on fission products while neutron cross sections are the main uncertainty contributors to the concentration of major actinides. Decay data has a negligible impact on isotopic

TABLE III. Relative uncertainty (in %) in number density on some major actinides and fission products at the end of the decay period.

Isotope	Decay	FY	XS	All
^{235}U	0.00	0.37	2.02	2.07
^{238}U	0.00	0.02	0.04	0.04
^{238}Pu	0.28	0.31	2.99	2.99
^{239}Pu	0.00	0.47	2.04	2.09
^{240}Pu	0.00	0.25	2.22	2.22
^{241}Pu	1.11	0.42	12.68	12.72
^{242}Pu	0.00	0.21	3.60	3.60
^{99}Tc	0.00	9.53	0.45	9.48
^{137}Cs	0.71	1.69	0.03	1.81
^{143}Nd	0.03	5.98	2.05	6.40
^{148}Nd	0.02	13.00	0.39	13.00
^{149}Sm	0.04	10.78	1.77	10.91
^{152}Sm	0.01	8.80	2.90	9.27

composition with some exceptions like ^{241}Pu (with a half-life of 14 years) and ^{137}Cs (30.2 years).

IV. CONCLUSIONS AND FUTURE DEVELOPMENTS

XSUSA was designed to assess the impact of nuclear data uncertainties on reactor core calculations. Until now, regarding nuclear data it has considered only cross section uncertainties. To complete the XSUSA propagation capabilities, a methodology was developed to generate decay and fission yields random libraries using the uncertainties found in ENDF/B-VII.1. The procedure has been applied to the UAM-6 burn-up pin-cell problem. It has been proved that the use of the varied libraries produce average k_{eff} results compatible with the reference values, included within the uncertainty coming from the nuclear data uncertainties. The impact of cross-sections and fission yields uncertainties is proved to be higher than the impact of decay constants both in criticality calculations and isotopic prediction.

The methodology must be extended to the use of different nuclear ENDF6-format data libraries in order to propagate their uncertainties. In future developments, concerning fission yields data, it should include correlation matrices in the varied fission yield libraries.

This work is the first step towards the completion of the XSUSA capability to propagate nuclear data uncertainties both jointly and independently. In order to benchmark the validity of the methodology, more realistic problems will be defined, for example, as a next step we envision the uncertainty assessment of complex scenarios involving full assembly models depleted up to a high burnup value in the framework of UAM-LWR (Phase II) project.

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